MM 24: Functional Materials II

Time: Tuesday 11:30–12:30 Location: H 1029

MM 24.1 Tue 11:30 H 1029

Tunable optical bandgap of polymeric carbon nitride photocatalysts — •Christoph Merschjann, Tobias Tyborski, Steven Orthmann, Florent Yang, Martha Christina Lux-Steiner, and Thomas Schedel-Niedrig — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Polymeric carbon nitrides with the approximate sum formula C_3N_4 have been shown to be photocatalytically active for hydrogen production from water under visible light illumination. For an effective sunlight-driven process, the bandgap of the catalyst should be in the range of 2 eV.

We have investigated the optical bandgap of carbon nitride polymers synthesized at different temperatures between 400 °C and 610 °C. The bandgaps are found to be linearly decreasing in the given temperature range, parallel to a decrease of the lattice constants of the polymer network. Thus, a tunability is given in the range $2.5\,\mathrm{eV} < E_\mathrm{g}^\mathrm{dir} < 3.0\,\mathrm{eV}$. Possible reasons for the observed effects are discussed in the presentation.

MM 24.2 Tue 11:45 H 1029

First-principles study of La–H: structural change from LaH_2 towards LaH_3 — •Tobias C. Kerscher[1,3], Gunther Schöllhammer[1], Walter Wolf[2], Stefan Müller[3], Peter Herzig[1], and Raimund Podloucky[1] — [1]University of Vienna, Institute of Physical Chemistry, Vienna, Austria — [2]Materials Design s.a.r.l., Le Mans, France — [3]Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Hamburg, Germany

By combination of first-principles density functional theory (DFT) and a cluster expansion (CE) with the UNCLE code [1], we investigate the interesting changes in the La–H system for the region between LaH_2 and LaH_3. These structural changes from the fluorite structure of the dihydride to the full trihydride drives a concentration-dependent metal-insulator transition ("switchable mirror") at $LaH_{\approx 2.8}$, as known by experiment. While our prior DFT study [2] had indeed already revealed the opening of a band gap at a hydrogen concentration close to LaH_3, we now show how a CE—based on input from DFT—predicts the structural changes in the full concentration range: It reveals the hydrogen's preference to occupy tetrahedral interstitial sites and the general formation of closely-paired hydrogen vacancies on octahedral interstitials. We compare our results to experiment.

[1] D. Lerch *et al.*, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009)

[2] G. Schöllhammer *et al.*, J. Alloys Comp. **480**, 111–113 (2009)

MM 24.3 Tue 12:00 H 1029

Systematic Study of the Hydrogen-Sensing Performance of Buffered and Capped Pd and PdNi Layers for Plasmonic Applications — •Nikolai Strohfeldt, Andreas Tittl, and Harald Giessen — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, D-70569 Stuttgart, Germany

We present a systematic experimental study of the hydrogen-sensing performance of buffered and capped Pd and PdNi layers. We focus specifically on the aging behavior of the thin films and compare the magnitude of the sensor response as well as the response time for freshly evaporated and 4 and 11 day old samples.

We find an optimized sample geometry consisting of a PdNi layer capped with 3 nm Pt and buffered with 10 nm of CaF_2 that exhibits excellent signal stability and linear signal response in the concentration range from 0.5% to 5% hydrogen in nitrogen.

The samples were measured in a custom-designed sensor head consisting of a light emitting diode and two photo-diodes that allow us to simultaneously track the reflected and transmitted light from our samples.

The observed insights can be easily incorporated into plasmonic geometries to improve concepts like antenna enhanced or perfect absorber based hydrogen sensing and allow us to move one step closer to a durable and industrially feasible optical plasmonic hydrogen sensor.

MM 24.4 Tue 12:15 H 1029

Hybrid Simulation of Nucleation Grow under External Forces — Robert Glöckner[1], Christian Heiliger[2], and •Stefan Kolling[1,3] — [1]Deutsches Kunststoff-Institut, Abt. Mechanik und Simulation, Darmstadt, Germany — [2]Justus Liebig Universität Gießen, I. Physikalisches Institut, Gießen, Germany — [3]Technische Hochschule Mittelhessen, Institut für Mechanik und Materialforschung, Gießen, Germany

Polymer (Polypropylene) nucleation grow and morphology dynamics under external forces are simulated by using hybrid simulation techniques.

The ambient phase and its properties are simulated using finite element methods in order to to accomplish for external forces like stress / strain / steady fluid-flow.

Nucleation grow is implemented as user-defined material within the FEM-solver using cellular automata (CA) to describe nucleation grow statisticaly.

Percolation algorithms are used to analyze evolving morphology of the system and provide graph-theoretic techniques for caching intermediate integrating results of the CA's in order to auto-detect areas of similiar behaviour (automatic symmetry detection).